

USER

HOST

DEVICE

[run.sh]

gpue <args>

[main]

[parseArgs()]

Parse arguments

[initialise()]

Setup host

Define **DEVICE** grid, block, and thread size

Calculate position and reciprocal space quantities

Allocate wavefunction, Hamiltonian, evolution operator memory blocks

Define initial wavefunction, Hamiltonian, evolution operators

[FileIO::writeOutXYZ()]

Write out to file

Open file and write

Free unnecessary memory

Allocate CUFFT plans

0

[FileIO::readIn()]

Read wavefunction from file

Open, read and write data to memory

wfc

-Copy **HOST** memory values to **DEVICE** memory-

[evolve]

Perform evolution

Initialise simulation variables

Print wavefunction at defined timesteps

[Tracker::vortPos()]

Track vortex position to nearest grid point

Locate +/- 2Pi phase windings

vortCoords

[Tracker::lsFit()]

Calculate accurate vortex position with least squares

Use 2x2 grid plaquettes to determine vortex position

vortCoords

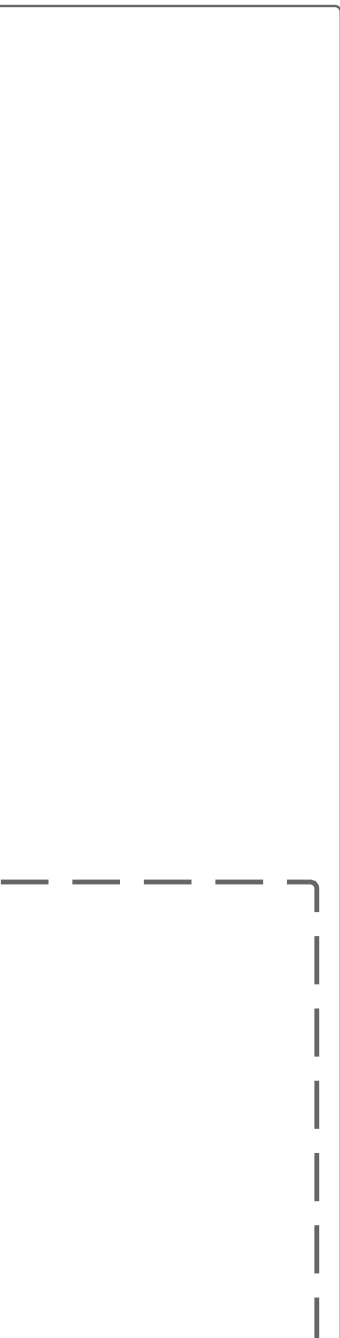
[Tracker::vortCentre()]

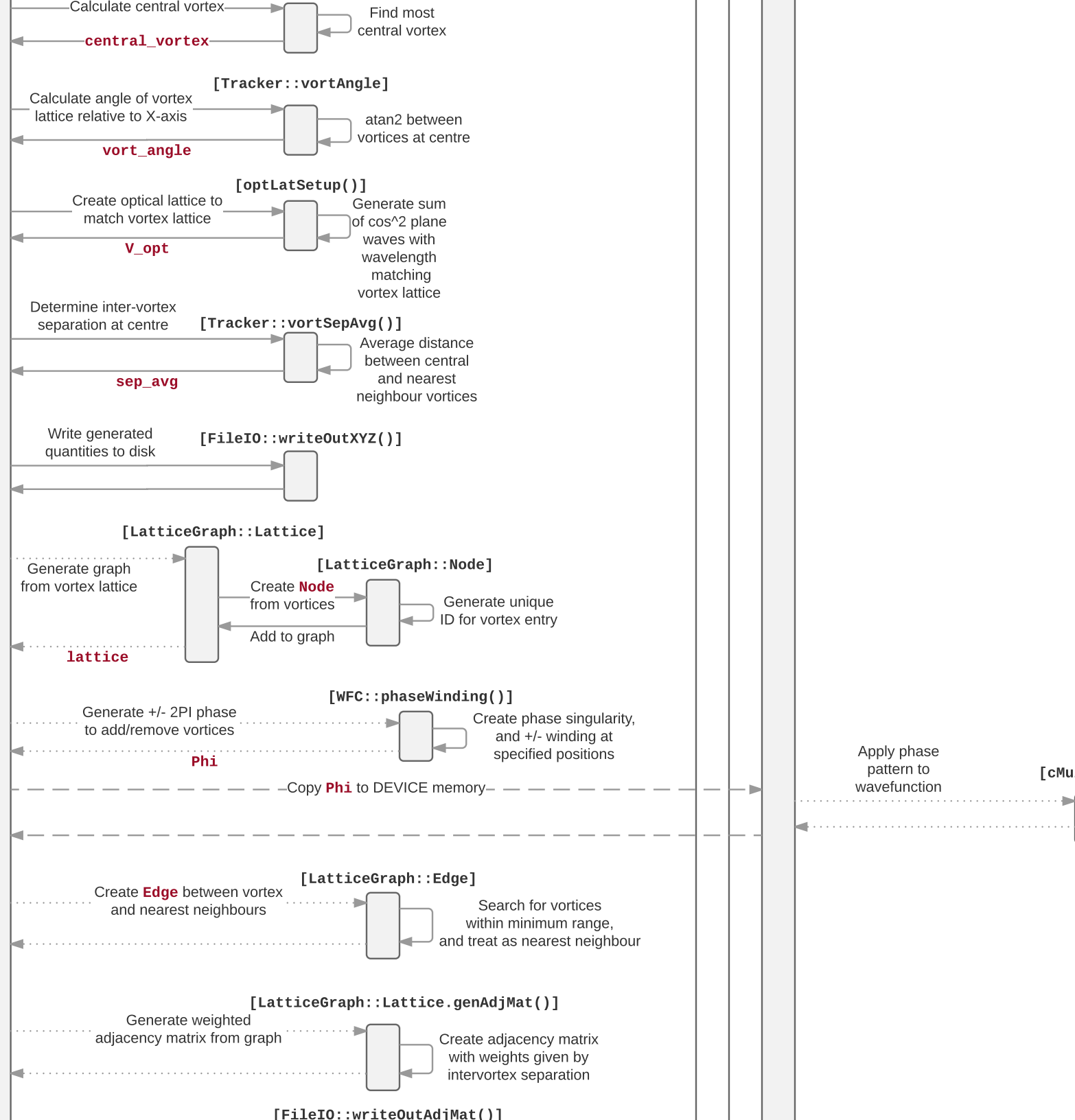
Calculate central vortex

Find most central vortex

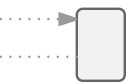
central_vortex

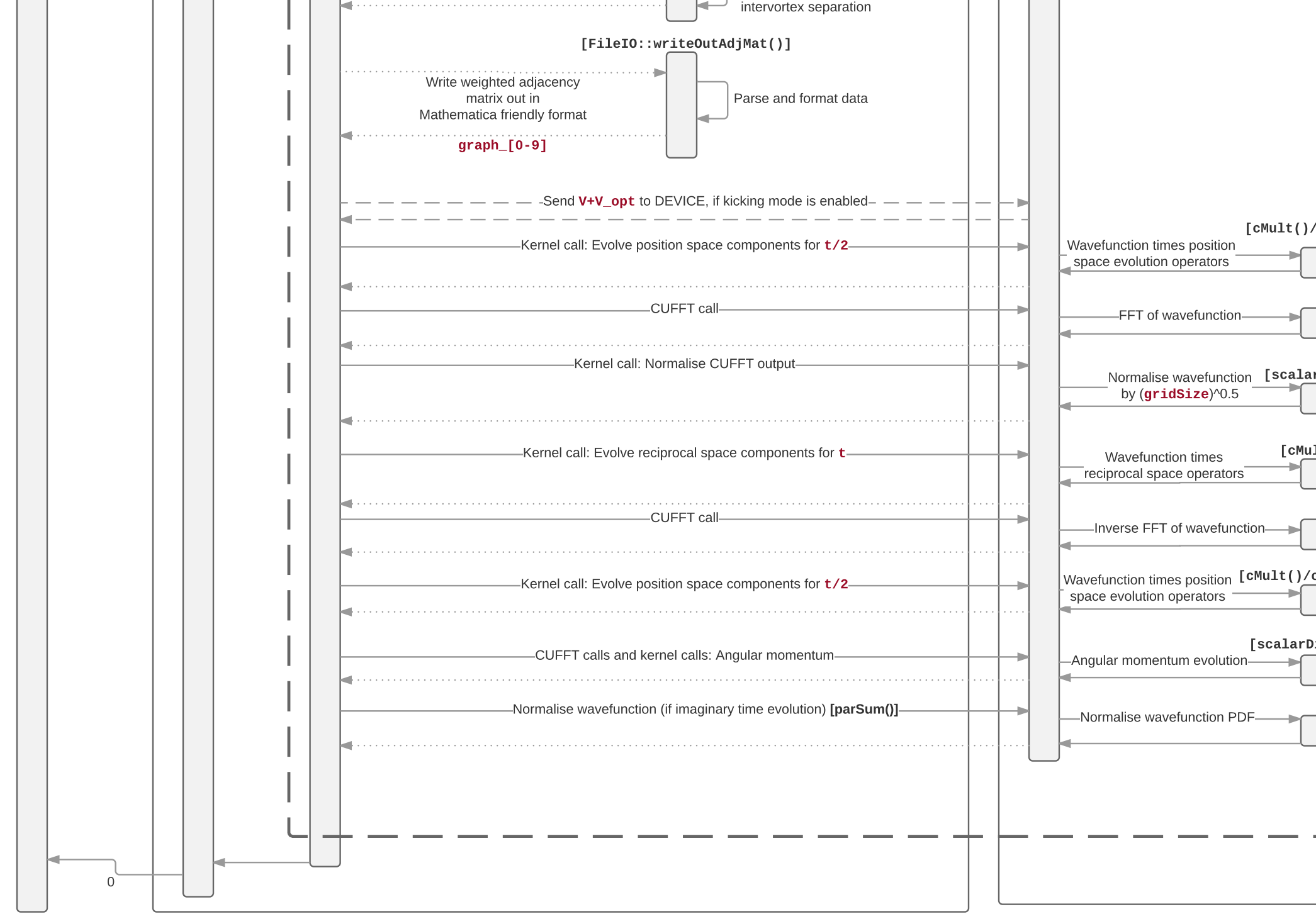
Evolution loop





[cMultPhi()]





`mult()/cMultDensity()`



`[scalarDiv()]`



`[cMult()]`



`mult()/cMultDensity()`



`scalarDiv(), angularOp()`

